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Poly[[(1,10-phenanthroline-κ^2N,N')cadmium(II)]-μ_3-pyridine-3,4-dicarboxylato-$\kappa^5N:O,O':O'',O'''$]

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Key indicators

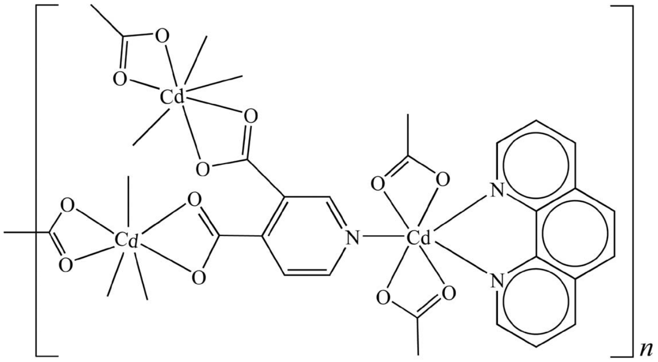
Single-crystal X-ray study
T = 283 K
Mean σ(C–C) = 0.005 Å
R factor = 0.031
wR factor = 0.094
Data-to-parameter ratio = 15.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Cd(C_7H_3NO_4)(C_{12}H_8N_2)]_n$, the Cd^{II} atom has a distorted pentagonal bipyramidal coordination geometry, defined by three N atoms and four carboxyl O atoms from chelating 1,10-phenanthroline and pyridine-3,4-dicarboxylate ligands. The structure exhibits a novel two-dimensional wave-like layer parallel to the (110) plane, with (6,3)-topology, which further forms a three-dimensional supramolecular network *via* π–π stacking.

Comment

In the last few years, the rational design and synthesis of metal–organic polymers has been of interest in the field of supramolecular chemistry and crystal engineering. The 3,4-pyridinedicarboxylate anion (PDB) has been investigated in the construction of metal–organic frameworks. Some structures of metal–organic polymers containing PDB have been reported previously (Wang, Qin, Wang, Li, Hao *et al.*, 2004; Wang, Qin, Wang, Li, Hu & Xu, 2004; Tong *et al.*, 2005; Zhang *et al.*, 2005; Chen *et al.*, 2003; Xia *et al.*, 2004; Qin *et al.*, 2005). Of these, two complexes, namely PDB-(2,2′-bipyridine)zinc(II) and PDB-(2,2′-bipyridine)cadmium(II), display a layered structure (Qin *et al.*, 2005). We present here the crystal structure of the title compound, (I), which is a new example of a compound with a layered polymeric structure.



(I)

As shown in Fig. 1, the asymmetric unit of (I) contains one Cd^{II} atom, one PDB and one 1,10-phenanthroline (phen) ligand. The Cd^{II} atom is coordinated by four O atoms from two PDB ligands and three N atoms from PDB and phen ligands, showing a distorted pentagonal bipyramidal coordination geometry. The distortion is considerable because of the small bite angles [O—Cd—O angles = 52.38 (8) and 53.23 (8)°] when PDB ligands coordinate with metal atoms. This is very different from the distorted square-pyramidal geometry found in PDB-(2,2′-bipyridine)cadmium(II) (Qin *et al.*, 2005). The Cd—O bond distances range from 2.262 (3) to 2.645 (3) Å, while the Cd—N bond distances range from 2.346 (3) to 2.388 (3) Å (Table 1).

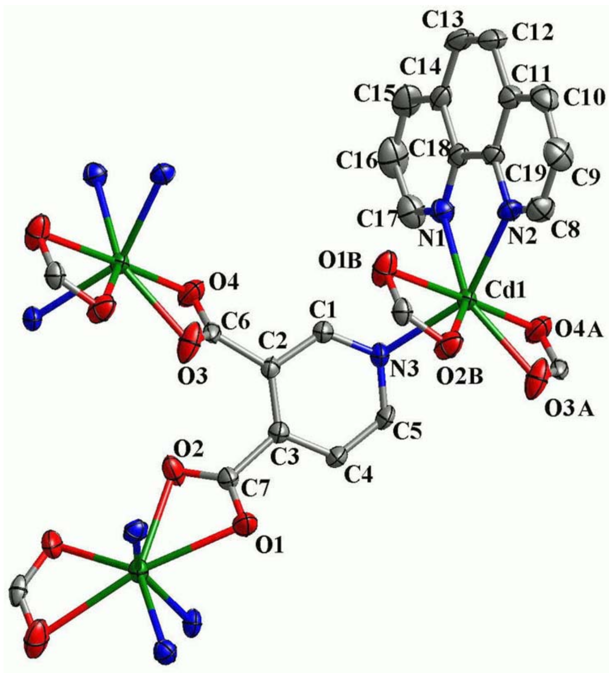


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and with 50% probability displacement ellipsoids. H atoms have been omitted. [Symmetry codes: (A) $1 + x, y, z$; (B) $-x, \frac{1}{2} + y, \frac{1}{2} - z$.]

Adjacent Cd^{II} atoms are linked by the PDB ligands to form a two-dimensional wave-like layer parallel to the (110) plane. Each PDB ligand serves as a three-connector, connecting three Cd^{II} atoms, while the Cd^{II} atom acts as a tri-connected node. The spontaneous association of these subunits results in a new kind of two-dimensional hexagonal (6,3) sheet, the three-connecting nodes of which are provided by both PDB^{2-} and Cd^{2+} (Fig. 2). The phen ligand chelates to the Cd^{II} atom in the direction nearly perpendicular to the two-dimensional layer. This orientation plays an important role in the packing. A three-dimensional network is formed *via* π–π stacking interactions between phen ligands, the face-to-face distances between neighbouring parallel phen planes being 3.436 (3) and 3.571 (3) Å (Fig. 3).

Experimental

Compound (I) was prepared by a hydrothermal method. A mixture of $Cd(NO_3)_2\cdot 6H_2O$ (0.5 mmol), H_2PDB (0.6 mmol) and water (10 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon reactor and kept at 433 K for 72 h under autogenous pressure. Single crystals of (I) suitable for X-ray analysis were obtained from the reaction mixture.

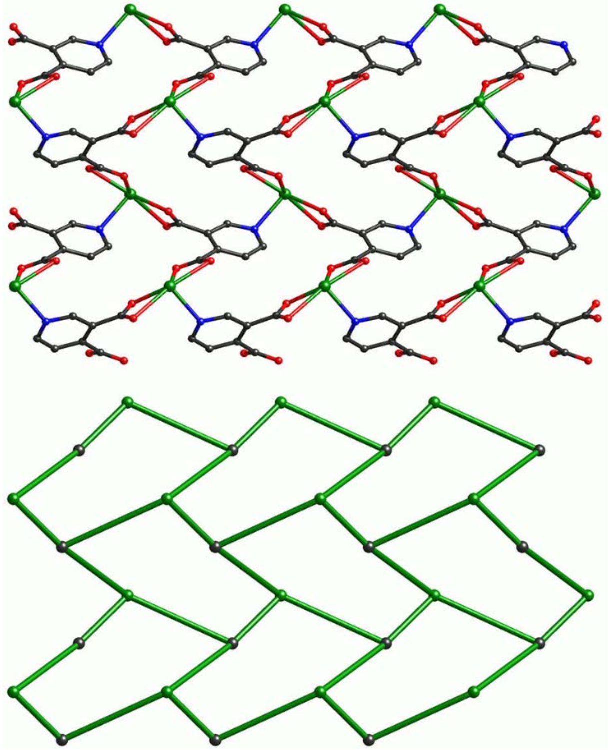


Figure 2
A perspective view of the two-dimensional layer, with phen ligands and H atoms omitted (top) and the (6,3) net (bottom).

Crystal data

$[Cd(C_7H_3NO_4)(C_{12}H_8N_2)]$
$M_r = 457.71$
Monoclinic, $P2_1/c$
$a = 7.5743$ (15) Å
$b = 9.4265$ (19) Å
$c = 23.070$ (5) Å
$\beta = 99.17$ (3)°
$V = 1626.1$ (6) Å^3
$Z = 4$

$D_x = 1.870$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15350 reflections
$\theta = 3.0$–27.5°
$\mu = 1.38$ mm^{-1}
$T = 283$ (2) K
Block, colourless
0.22 × 0.20 × 0.16 mm

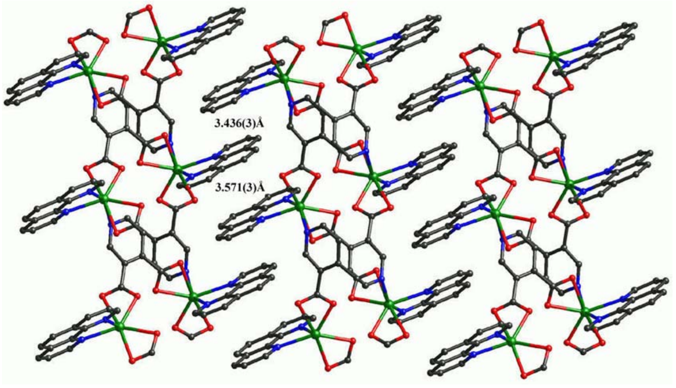


Figure 3
A packing model of the three-dimensional supramolecular network. H atoms have been omitted.

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Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.752$, $T_{\max} = 0.810$
15350 measured reflections

3700 independent reflections
3190 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -27 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.094$
$S = 1.01$
3700 reflections
244 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.473P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.65$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.360 (3)	Cd1—O2$^{\rm i}$	2.406 (2)
Cd1—N2	2.346 (3)	Cd1—O3$^{\rm ii}$	2.262 (3)
Cd1—N3	2.388 (3)	Cd1—O4$^{\rm ii}$	2.645 (3)
Cd1—O1$^{\rm i}$	2.494 (3)		

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x + 1, y, z$.

The H atoms were placed in calculated positions, with C—H = 0.93 Å, and treated as riding atoms in the final cycles of refinement, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *SHELXL97*.

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